Full wwPDB EM Validation Report (i)

Aug 7, 2023 – 03:30 PM EDT

PDB ID	:	5VHF
EMDB ID	:	EMD-8674
Title	:	Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle
Authors	:	Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on	:	2017-04-13
Resolution	:	5.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

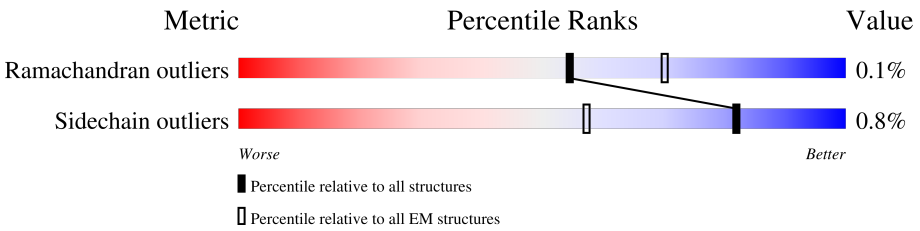
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	223	95% 98% •
2	A	352	74% 97% •
3	B	340	78% 96% • •
4	C	385	65% 88% • 11%
5	D	368	67% 93% • 7%
6	E	379	65% 90% • 9%
7	F	380	67% 93% • 6%
8	U	841	15% 89% 11%
9	V	183	28% 100%

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Mol	Chain	Length	Quality of chain
10	W	456	31% 99%
11	X	385	40% 100%
12	Y	378	18% 100%
13	Z	286	26% 100%
14	a	374	23% 100%
15	b	191	24% 99%
16	c	287	20% 100%
17	d	136	44% 99%
18	e	70	39% 100%
19	f	848	76% 79% 19%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 51096 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S proteasome non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	219	1662	1036	294	323	9	0	0

- Molecule 2 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	341	2677	1690	473	497	17	0	0

- Molecule 3 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	330	2579	1624	437	506	12	0	0

- Molecule 4 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	342	2709	1701	493	501	14	0	0

- Molecule 5 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	344	2751	1744	480	517	10	0	0

- Molecule 6 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	345	2736	1715	490	515	16	0	0

- Molecule 7 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	359	2808	1772	488	531	17	0	0

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	U	751	5829	3696	1001	1088	44	0	0

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	V	183	1480	949	260	265	6	0	0

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	W	456	3703	2339	635	704	25	0	0

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	X	385	3048	1939	515	582	12	0	0

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Y	378	3115	1987	533	578	17	0	0

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Z	286	2281	1457	392	427	5	0	0

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	a	374	3003	1915	511	562	15	0	0

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	b	191	1458	910	261	279	8	0	0

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	c	287	2260	1430	389	422	19	0	0

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	d	136	1109	720	176	209	4	0	0

- Molecule 18 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	e	70	583	357	89	135	2	0	0

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	f	686	5304	3335	901	1033	35	0	0

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

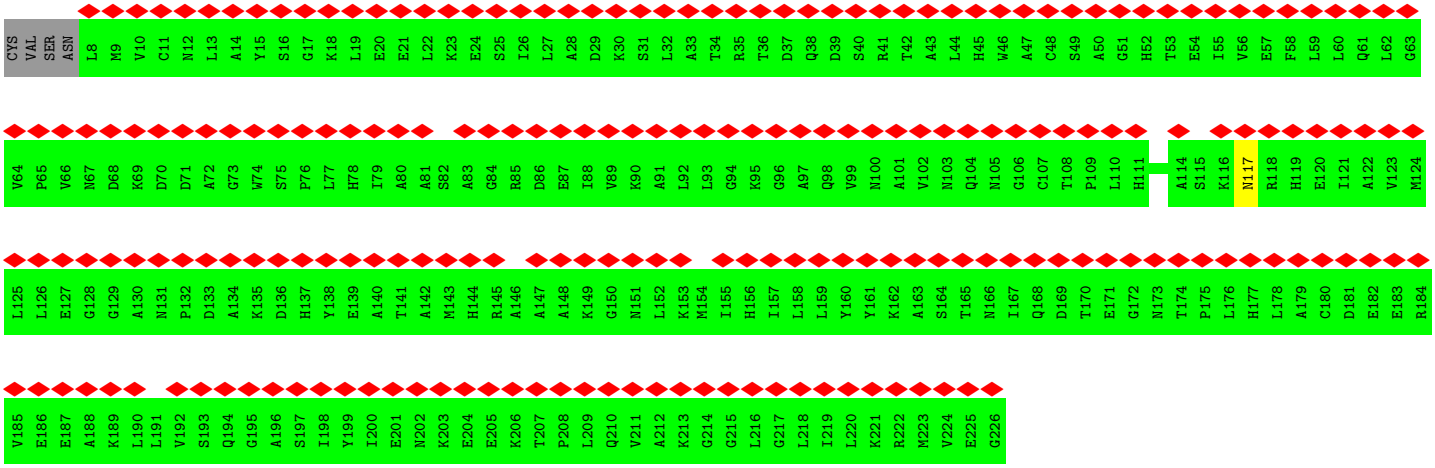
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	c	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

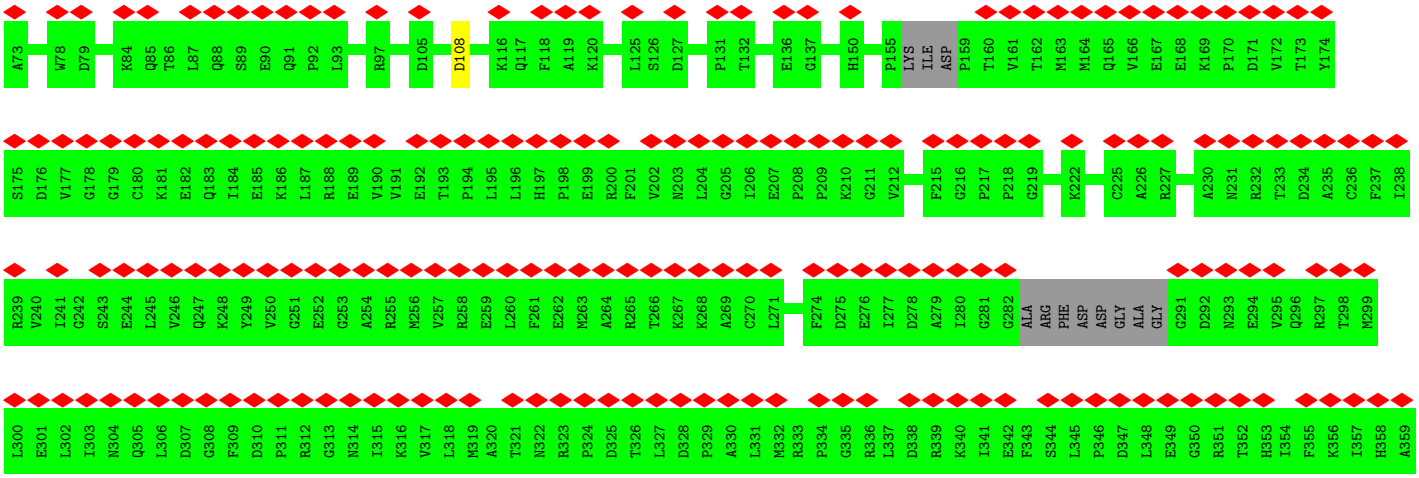
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 10

Chain G: 95% 98%



- Molecule 2: 26S proteasome regulatory subunit 7

Chain A: 74% 97%



R360 S361 M362 S363 V364 E365 R366 D367 I368 R369 F370 E371 L372 L373 A374 R375 L376 C377 P378 N379 S380 T381 G382 A383 E384 I385 R386 S387 V388 C389 T390 E391 A392 G393 M394 F395 A396 I397 R398 A399 R400 R401 K402 I403 A404 T405 E406 K407 D408 F409 L410 E411 A412 V413 N414 K415 V416 I417 K418 S419

Y420 A421 K422 F423 S424

• Molecule 3: 26S proteasome regulatory subunit 4

Chain B: 78% 96%

E93 E94 E95 D100 D101 S108 L112 D117 S126 V127 I135 K141 D142 L143 L144 E145 S149 V150 L151 L152 N153 H154 K155 G161 V162 L163 M164 D165 ASP THR D168 P169 L170 V171 T172 V173 M174 K175 V176 E177 K178 A179 P180 Q181 E182 T183 Y184 A185 D186 I187 G188

G189 L190 D191 N192 Q193 I194 Q195 E196 I197 K198 E199 S200 V201 E202 L203 P204 L205 T206 H207 P208 E209 Y210 Y211 E212 E213 M214 G215 I216 K217 P218 P219 K220 G221 V222 I223 L224 Y225 G226 P227 P228 G229 T230 G231 K232 T233 L234 L235 A236 K237 A238 V239 A240 N241 Q242 T243 S244 A245 T246 F247 L248

R249 V250 V251 G252 S253 E254 L255 I256 Q257 K258 Y259 L260 G261 D262 G263 P264 K265 L266 V267 R268 E269 L270 F271 R272 V273 A274 E275 E276 H277 A278 P279 S280 I281 V282 F283 I284 D285 E286 I287 D288 A289 I290 G291 T292 LYS ARG TYR ASP SER ASN SER GLY G301 E302 R303 E304 I305 Q306 R307 T308

M309 L310 E311 L312 L313 N314 Q315 L316 D317 G318 F319 D320 S321 R322 G323 D324 V325 K326 M329 A330 T331 N332 R333 I334 E335 T336 L337 D338 P339 A340 L341 I342 R343 P344 G345 R346 I347 D348 R349 K350 I351 E352 F353 P354 L355 P356 D357 E358 K359 T360 K361 K362 R363 I364 F365 Q366 I367 H368 T369

S370 R371 M372 T373 L374 A375 D376 D377 V378 T379 L380 D381 D382 L383 I384 M385 A386 K387 D388 D389 L390 S391 G392 A393 D394 I395 K396 A397 I398 C399 T400 E401 A402 G403 L404 M405 A406 L407 R408 E409 R410 R411 M412 K413 V414 T415 N416 E417 D418 F419 K420 K421 S422 K423 E424 N425 V426 L427 Y428 K429

K430 Q431 E432

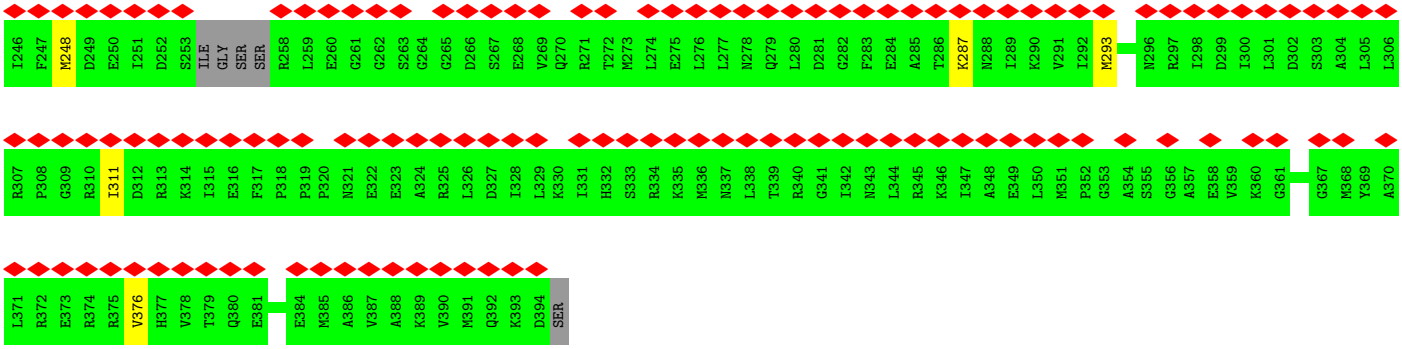
• Molecule 4: 26S proteasome regulatory subunit 8

Chain C: 65% 88% 11%

L11 E12 K15 A16 R44 E61 L65 L66 Q67 E68 Q69 Y72 V73 G74 E75 V76 A79 M80 D81 K82 K83 K84 V85 L86 V87 K88 V89 H90 P91 E92 G93 K94 V99 D100 K101 N102 I103 D104 I105 N106 D107 V108 T109 P110 N111 C112 R113 R117 N118 L123 H124

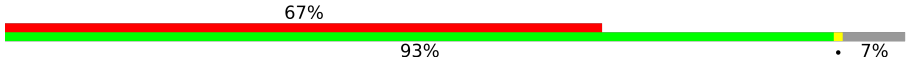
K125 I126 L127 P128 ASN LYS VAL ASP PRO LEU VAL SER LEU MET MET VAL GLU LYS VAL PRO ASP SER THR TYR GLU MET ILE GLY GLY L154 D155 K156 Q157 I158 K159 E160 I161 K162 E163 V164 I165 E166 L167 P168 V169 K170 H171 P172 E173 L174 F175 E176 A177 L178 G179 I180 A181 Q182 P183 K184

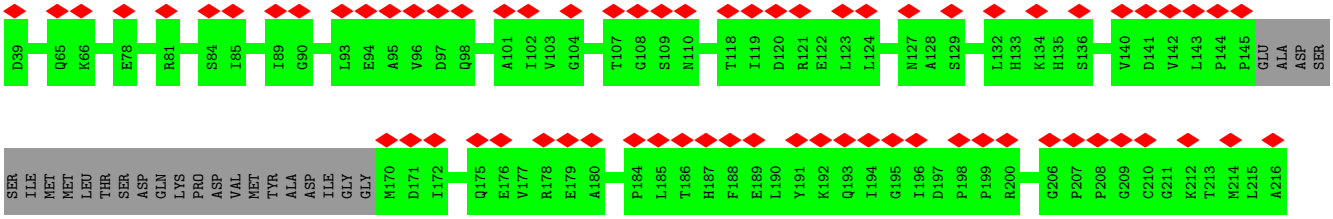
G185 V186 L187 L188 Y189 G190 P191 P192 G195 K196 T197 L198 L199 A200 R201 A202 V203 A204 H205 H206 T207 D208 C209 T210 F211 I212 R213 V214 S215 GLY SER GLU GLU LEU VAL GLN LYS PHE ILE GLY GLU GLY ALA R229 M230 V231 R232 E233 L234 F235 V236 M237 A238 R239 E240 H241 A242 P243 S244 I245

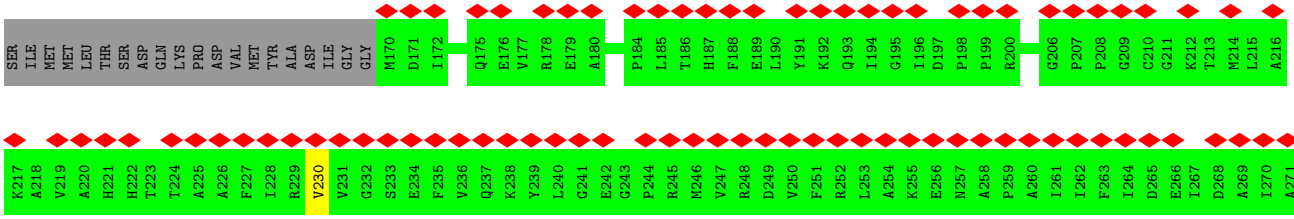


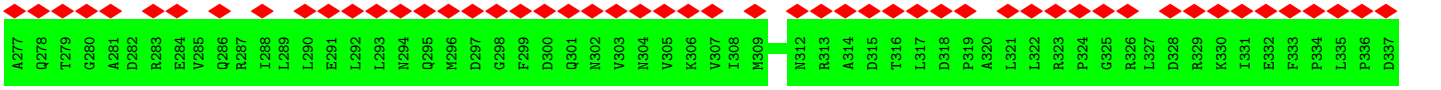
- Molecule 5: 26S proteasome regulatory subunit 6B

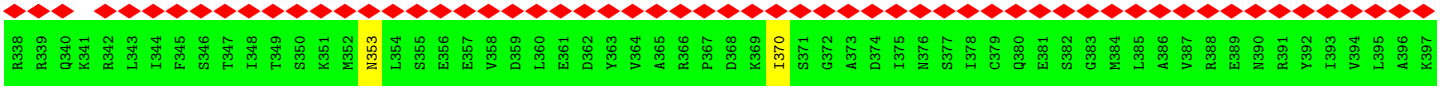
Chain D:

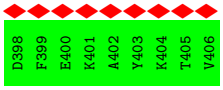






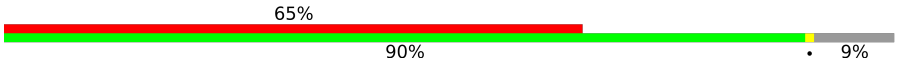


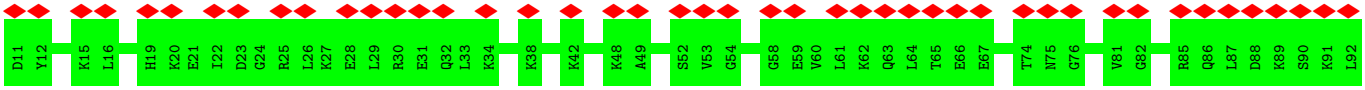


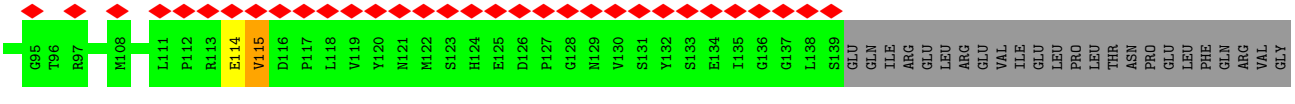


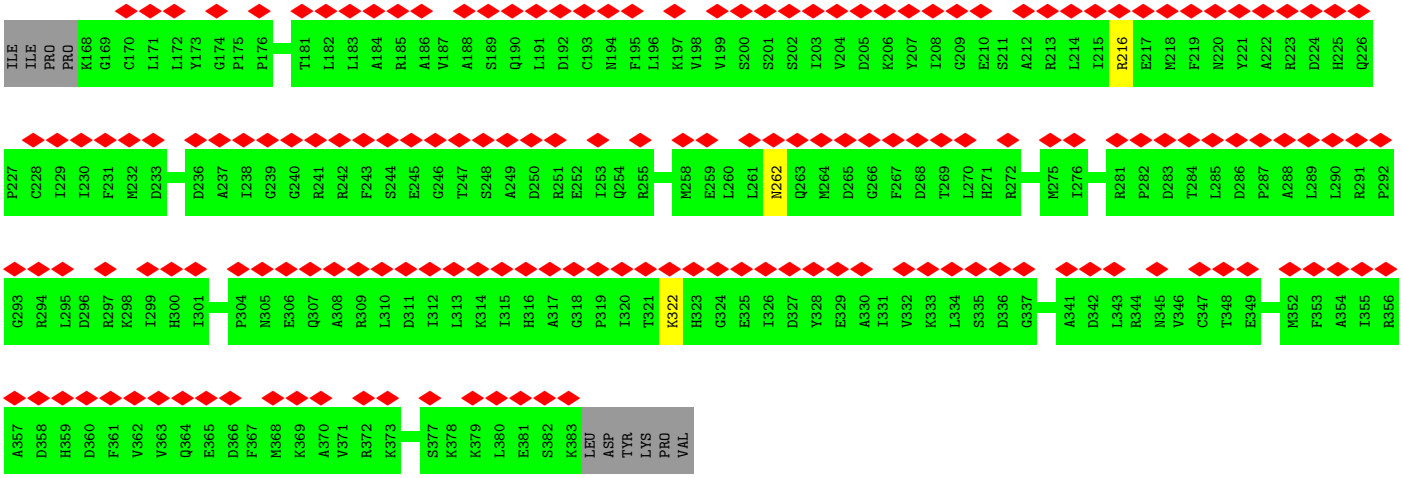
- Molecule 6: 26S proteasome regulatory subunit 10B

Chain E:



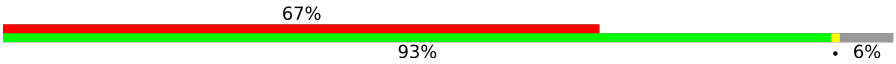


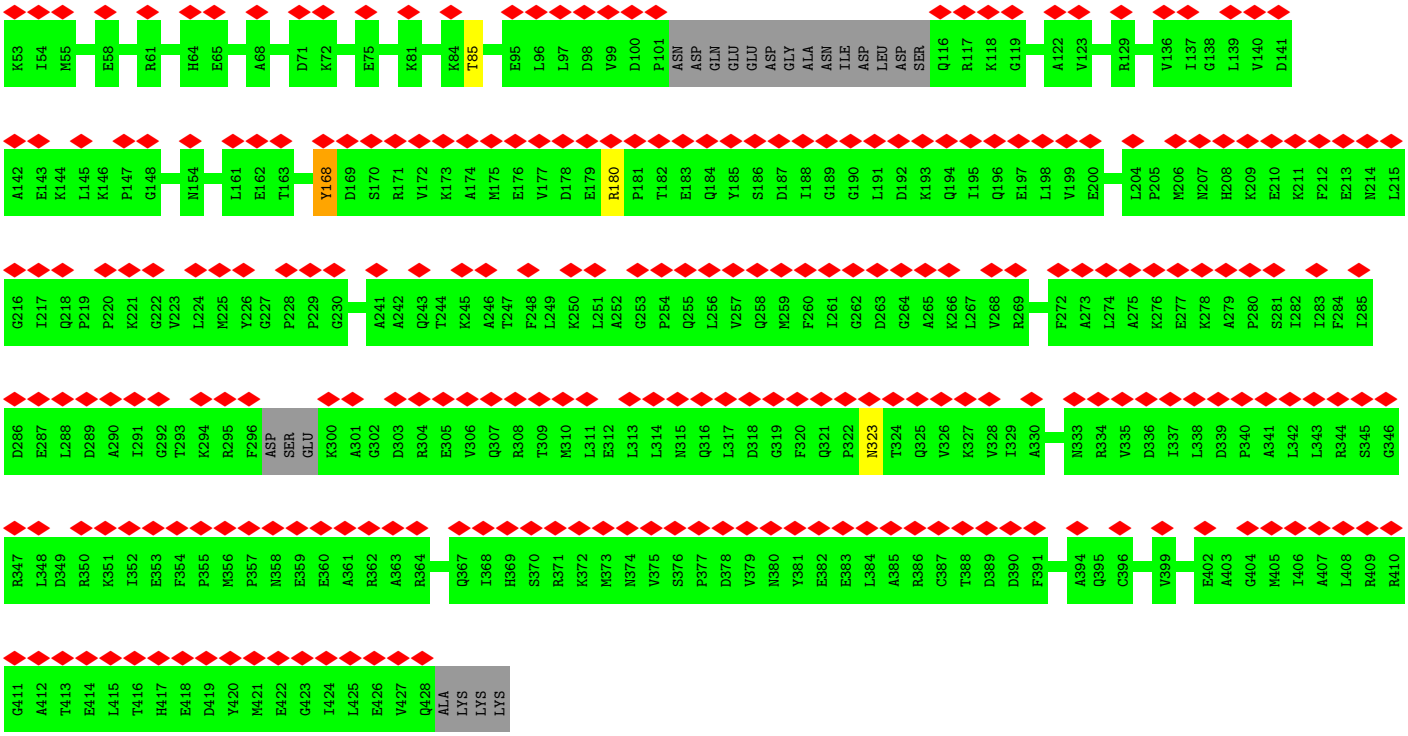




- Molecule 7: 26S proteasome regulatory subunit 6A

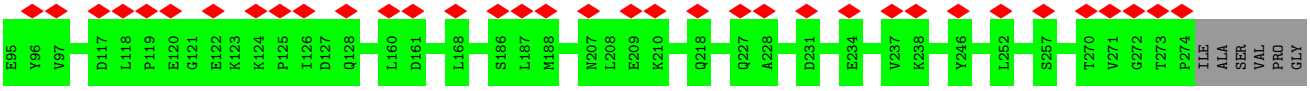
Chain F:

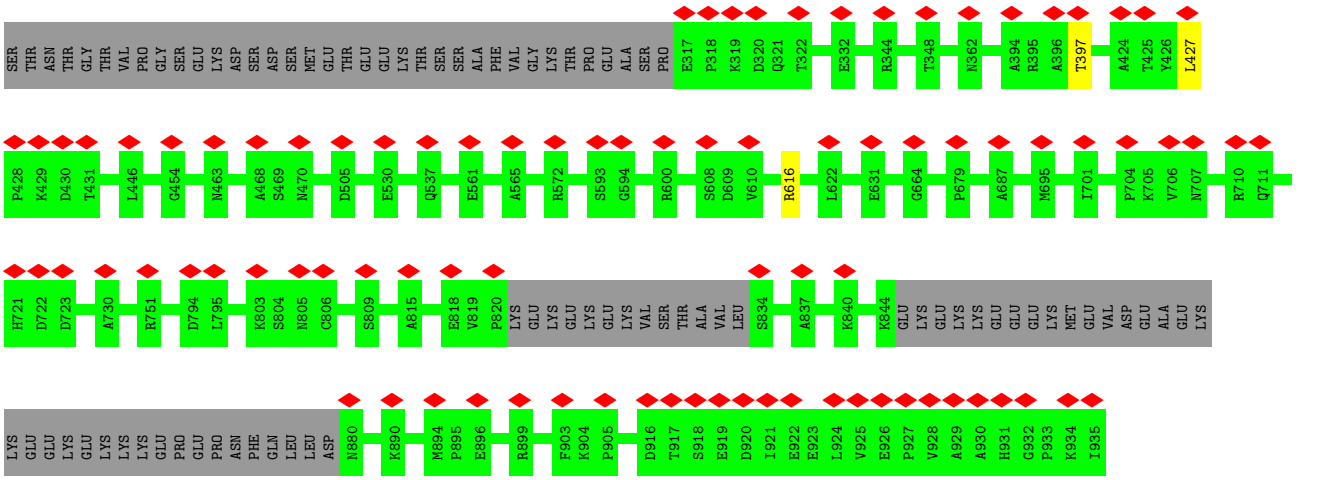




- Molecule 8: 26S proteasome non-ATPase regulatory subunit 1

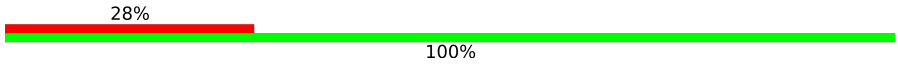
Chain U:

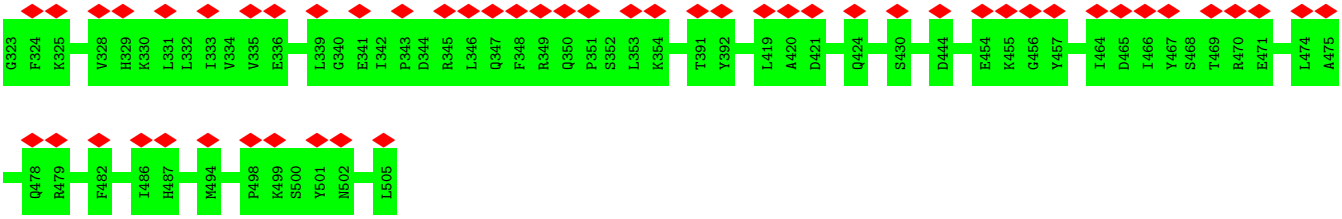




- Molecule 9: 26S proteasome non-ATPase regulatory subunit 3

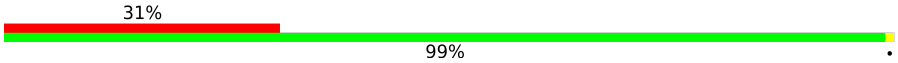
Chain V:

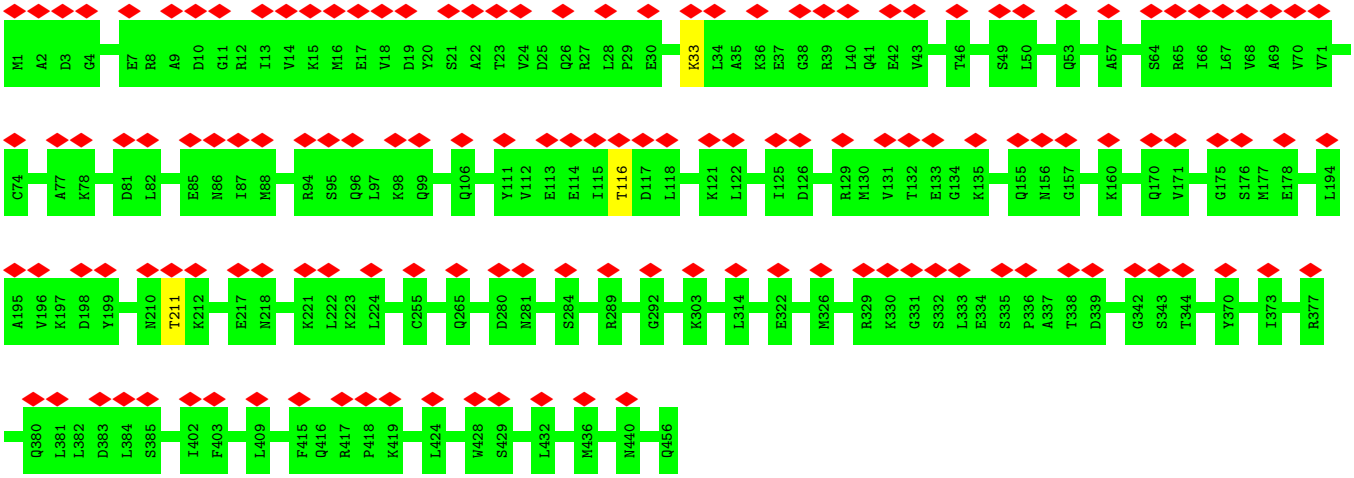




- Molecule 10: 26S proteasome non-ATPase regulatory subunit 12

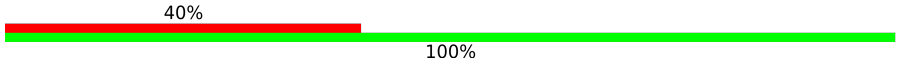
Chain W:

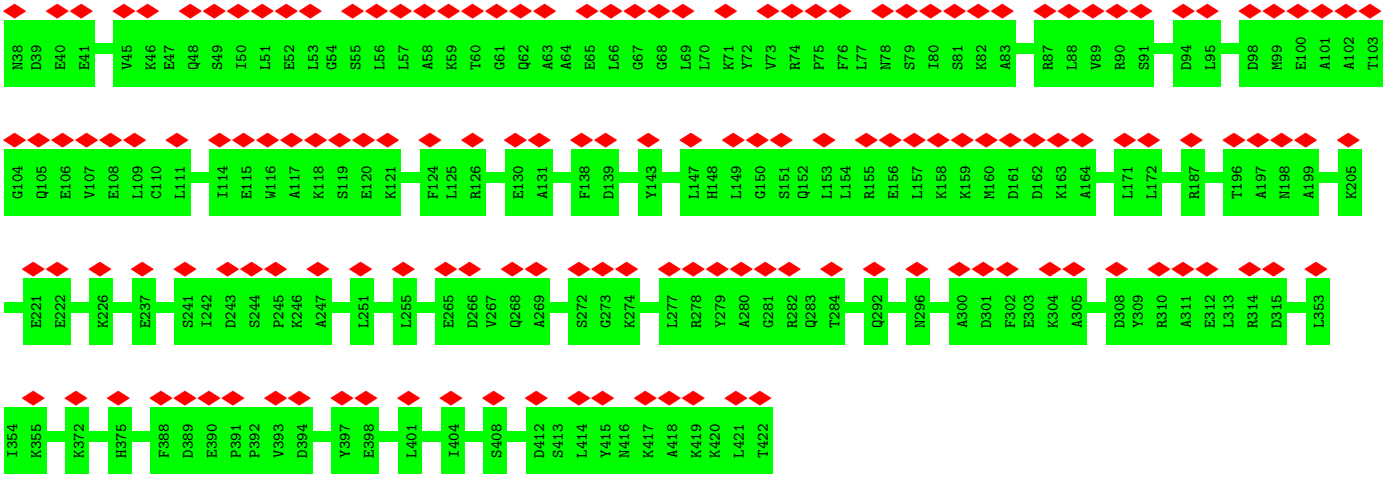




- Molecule 11: 26S proteasome non-ATPase regulatory subunit 11

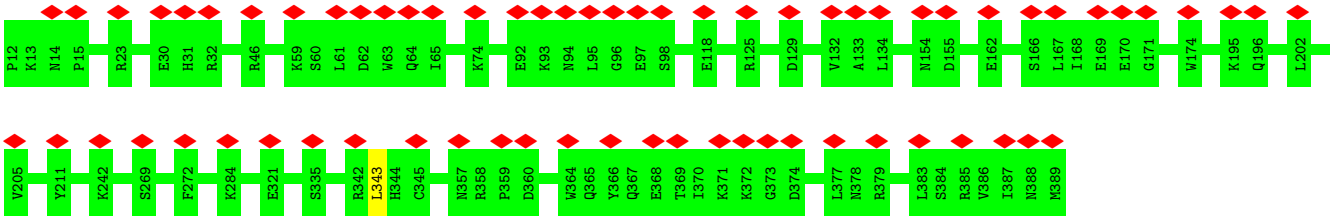
Chain X:





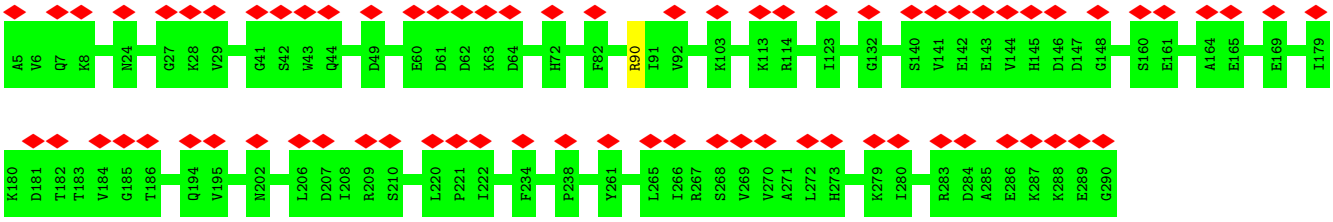
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 18% 100%



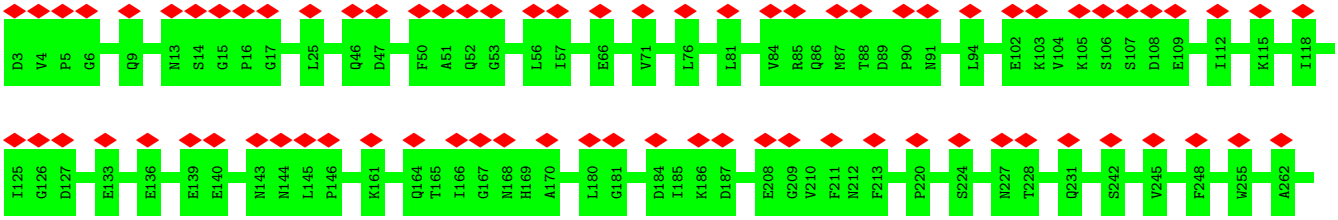
- Molecule 13: 26S proteasome non-ATPase regulatory subunit 7

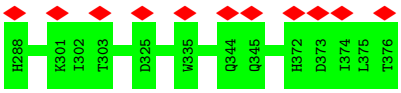
Chain Z: 26% 100%



- Molecule 14: 26S proteasome non-ATPase regulatory subunit 13

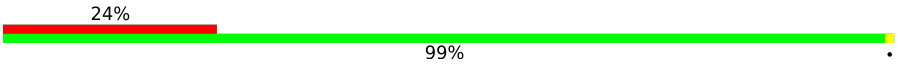
Chain a: 23% 100%

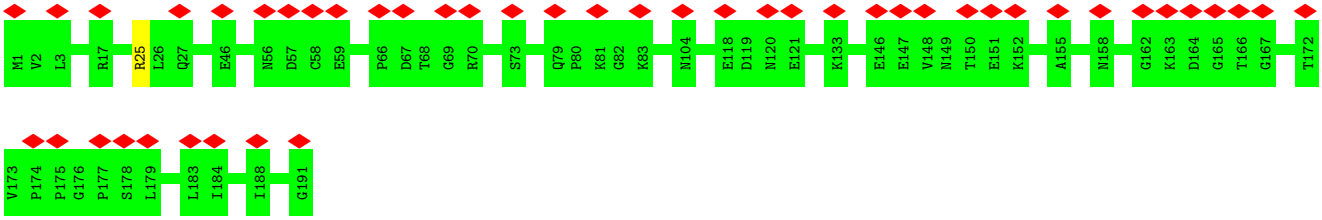




• Molecule 15: 26S proteasome non-ATPase regulatory subunit 4

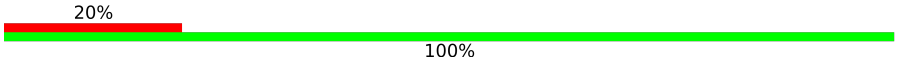
Chain b:

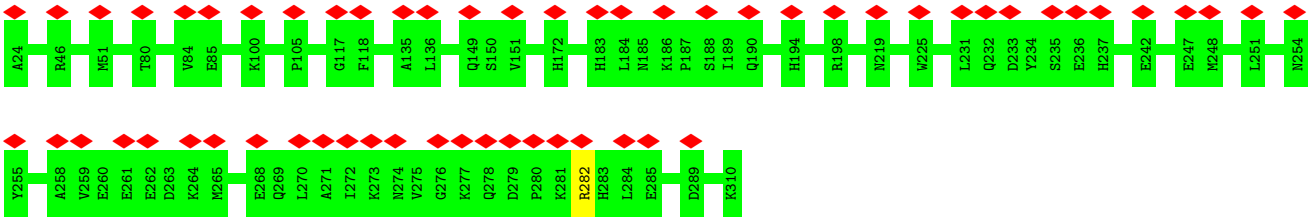




• Molecule 16: 26S proteasome non-ATPase regulatory subunit 14

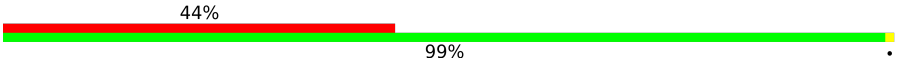
Chain c:

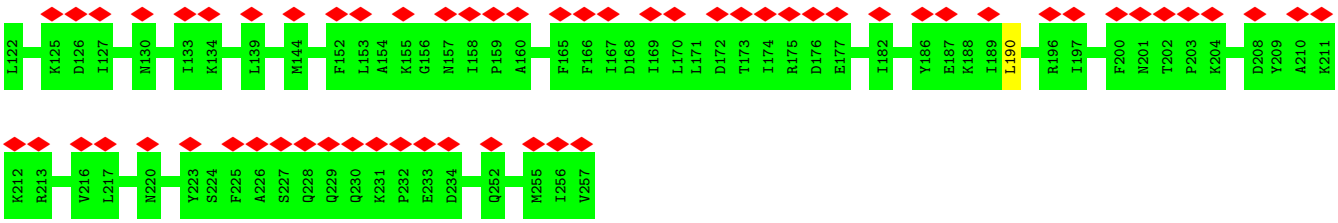




• Molecule 17: 26S proteasome non-ATPase regulatory subunit 8

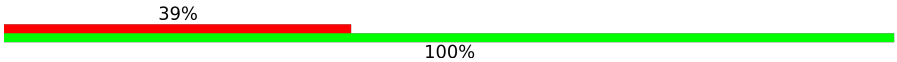
Chain d:

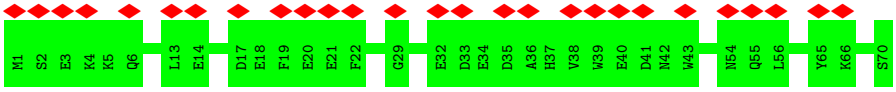




• Molecule 18: 26S proteasome complex subunit SEM1

Chain e:





• Molecule 19: 26S proteasome non-ATPase regulatory subunit 2

Chain f:

R6 D7 K8 A9 P10 V11 Q12 P13 Q14 Q15 S16 P17 A18 A19 A20 P21 G22 G23 T24 D25 E26 K27 P28 S29 G30 K31 E32 R33 R34 D35 A36 G37 D38 K39 D40 K41 E42 Q43 E44 L45 S46 E47 E48 D49 K50 Q51 L52 Q53 D54 E55 LEU GLU MET LEU LEU VAL GLU ARG LEU GLY GLU

LYS ASP THR SER L70 Y71 R72 P73 A74 L75 E76 E77 L78 R79 R80 Q81 I82 R83 S84 S85 T86 T87 S88 M89 T90 S91 V92 P93 K94 P95 L96 K97 F98 L99 R100 P101 H102 Y103 GLY LYS LEU LYS GLU ILE TYR GLU ASN MET ALA PRO GLY GLU N118 K119 R120 F121 A122 A123 D124 I125

I126 S127 V128 L129 A130 M131 T132 M133 S134 G135 E136 R137 E138 C139 L140 K141 Y142 R143 L144 V145 G146 SER GLN GLU GLU LEU ALA SER TRP GLY HIS GLU TYR VAL ARG HIS LEU A163 G164 E165 V166 A167 K168 E169 W170 Q171 E172 L173 D174 D175 A176 E177 K178 V179 Q180 R181 E182 P183 L184 L185

T186 L187 V188 K189 E190 I191 V192 P193 TYR ASN MET ALA HIS ASN ALA GLU HIS GLU ALA CYS ASP L207 L208 M209 E210 I211 E212 Q213 V214 D215 M216 L217 E218 K219 D220 I221 D222 E223 N224 A225 Y226 A227 K228 V229 C230 L231 Y232 L233 T234 S235 C236 V237 N238 Y239 V240 P241 E242 P243 E244 N245

S246 A247 L248 L249 R250 C251 A252 L253 G254 V255 F256 R257 K258 F259 S260 R261 F262 P263 E264 A265 L266 R267 L268 A269 L270 M271 L272 N273 D274 M275 E276 L277 V278 E279 D280 I281 F282 T283 S284 C285 K286 D287 V288 V289 VAL GLN LYS GLN MET ALA PHE M297 L298 G299 R300 H301 G302 V303 F304 L305

E306 L307 S308 V311 E312 E313 Y314 E315 D316 L317 T318 E319 I320 M321 S322 N323 V324 Q325 L326 N327 S328 N329 F330 L331 A332 L333 A334 R335 E336 L337 D338 I339 M340 E341 P342 K343 V344 P345 D346 D347 I348 Y349 K350 T351 H352 L353 E354 N355 N356 R357 F358 G359 G360 S361 G362 S363 Q364 V365 D366

S367 A368 R369 M370 N371 L372 A373 S374 S375 F376 V377 N378 G379 F380 V381 N382 ALA ALA PHE GLY Q387 D388 K389 L390 L391 T392 D393 D394 G395 N396 K397 W398 L399 Y400 K401 N402 K403 D404 H405 G406 M407 L408 S409 A410 A411 A412 S413 L414 G415 M416 I417 L418 L419 W420 D421 V422 D423 G424 G425 L426

T427 Q428 I429 D430 K431 Y432 L433 Y434 S435 S436 E437 D438 Y439 I440 K441 S442 G443 A444 L445 L446 A447 C448 G449 I450 V451 G454 V455 R456 N457 E458 C459 D460 P461 A462 L463 A464 L465 L466 S467 D468 Y469 V470 L471 H472 N473 S474 N475 T476 M477 R478 L479 G480 S481 I482 F483 G484 L485 G486 L487

A488 Y489 ALA GLY SER N493 R494 E495 D496 V497 L498 T499 L500 L501 L502 P503 V504 M505 G506 D507 S508 K509 S510 S511 M512 E513 V514 A515 G516 V517 T518 A519 L520 A521 A526 V527 G528 S529 C530 N531 G532 D533 V534 T535 S536 T537 I538 L539 Q540 T541 I542 M543 E544 K545 S546 E547 T548 E549 L550

K551 D552 T553 Y554 A555 R556 W557 L558 P559 L560 G561 L562 G563 L564 N565 H566 L567 G568 K569 G570 E571 A572 I573 E574 A575 I576 L577 A578 A579 L580 E581 V582 V583 S584 E585 P586 F587 R588 S589 F590 A591 N592 T593 L594 V595 D596 V597 C598 A599 Y600 S603 G604 N605 V606 L607 K608 V609 Q610 D611

L612 L613 H614 S617 E618 H619 F620 D621 S622 K623 E624 K625 E626 E627 D628 K629 D630 K631 K632 E633 K634 K635 D636 K637 D638 K639 K640 E641 A642 P643 A644 D645 M646 G647 A648 H649 Q650 G651 V652 A653 V654 L655 G656 I657 A658 L659 I660 A661 M662 G663 E664 E665 I666 G667 A668 E669 M670 A671 L672

R673 T674 F675 G676 H677 L678 H679 R680 Y681 G682 E683 P684 T685 L686 R687 R688 A689 V690 P691 L692 A693 L694 A695 L696 I697 S698 V699 SER ASN PRO ARG LEU ASN ILE LEU ASP THR LEU SER LYS PHE S714 H715 D716 A717 D718 P719 E720 V721 S722 Y723 N724 S725 I726 F727 A728 MET GLY MET VAL

GLY SER GLY THR ASN ASN A739 R740 L741 A742 A743 M744 L745 R746 Q747 L748 A749 Q750 Y751 H752 A753 K754 ASP PRO ASN ASN LEU PHE MET VAL ARG LEU ALA GLN GLY LEU THR HIS LEU GLY K773 G774 T775 L776 T777 L778 C779 P780 Y781 H782 S783 D784 R785 Q786 L787 M788 S789 Q790 V791 A792

V793 A794 G795 L796 L797 T798 V799 L800 V801 S802 F803 L804 ASP VAL ARG ASN ILE ILE LEU GLY LYS SER HIS TYR VAL LEU TYR GLY LEU VAL ALA ALA MET GLN PRO ARG MET LEU VAL THR PHE ASP GLU GLU LEU ARG PRO LEU PRO VAL SER VAL ARG VAL GLY GLN ALA VAL ASP VAL

VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.012	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	250.88, 250.88, 250.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	G	0.23	0/1687	0.37	0/2279
2	A	0.23	0/2722	0.42	0/3673
3	B	0.23	0/2615	0.44	0/3530
4	C	0.23	0/2741	0.39	0/3681
5	D	0.24	0/2795	0.42	0/3773
6	E	0.32	2/2775 (0.1%)	0.47	3/3727 (0.1%)
7	F	0.24	0/2845	0.42	0/3832
8	U	0.23	0/5930	0.40	0/8021
9	V	0.24	0/1507	0.39	0/2029
10	W	0.23	0/3750	0.39	0/5039
11	X	0.23	0/3091	0.36	0/4165
12	Y	0.23	0/3173	0.37	0/4273
13	Z	0.23	0/2324	0.39	0/3150
14	a	0.23	0/3061	0.38	0/4144
15	b	0.23	0/1478	0.40	0/2001
16	c	0.23	0/2302	0.38	0/3110
17	d	0.24	0/1134	0.39	0/1534
18	e	0.23	0/596	0.40	0/805
19	f	0.24	0/5377	0.42	0/7248
All	All	0.24	2/51903 (0.0%)	0.40	3/70014 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	115	VAL	N-CA	8.47	1.63	1.46
6	E	115	VAL	CA-C	5.87	1.68	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	115	VAL	C-N-CA	-8.17	101.28	121.70
6	E	115	VAL	CA-C-N	7.58	133.87	117.20
6	E	115	VAL	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	217/223 (97%)	214 (99%)	3 (1%)	0	100	100
2	A	335/352 (95%)	301 (90%)	34 (10%)	0	100	100
3	B	326/340 (96%)	294 (90%)	30 (9%)	2 (1%)	25	65
4	C	334/385 (87%)	313 (94%)	21 (6%)	0	100	100
5	D	340/368 (92%)	317 (93%)	23 (7%)	0	100	100
6	E	341/379 (90%)	311 (91%)	28 (8%)	2 (1%)	25	65
7	F	353/380 (93%)	329 (93%)	23 (6%)	1 (0%)	41	76
8	U	743/841 (88%)	714 (96%)	29 (4%)	0	100	100
9	V	181/183 (99%)	170 (94%)	11 (6%)	0	100	100
10	W	452/456 (99%)	414 (92%)	38 (8%)	0	100	100
11	X	381/385 (99%)	375 (98%)	6 (2%)	0	100	100
12	Y	376/378 (100%)	357 (95%)	19 (5%)	0	100	100
13	Z	284/286 (99%)	267 (94%)	17 (6%)	0	100	100
14	a	372/374 (100%)	351 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	b	189/191 (99%)	174 (92%)	15 (8%)	0	100	100
16	c	285/287 (99%)	271 (95%)	14 (5%)	0	100	100
17	d	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
18	e	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
19	f	664/848 (78%)	597 (90%)	67 (10%)	0	100	100
All	All	6375/6862 (93%)	5956 (93%)	414 (6%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	169	PRO
3	B	168	ASP
7	F	168	TYR
6	E	114	GLU
6	E	115	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	174/178 (98%)	173 (99%)	1 (1%)	86	92
2	A	293/300 (98%)	292 (100%)	1 (0%)	92	94
3	B	289/298 (97%)	286 (99%)	3 (1%)	76	86
4	C	297/333 (89%)	292 (98%)	5 (2%)	60	78
5	D	301/321 (94%)	298 (99%)	3 (1%)	76	86
6	E	300/333 (90%)	297 (99%)	3 (1%)	76	86
7	F	308/326 (94%)	304 (99%)	4 (1%)	69	82
8	U	639/720 (89%)	636 (100%)	3 (0%)	88	93
9	V	164/164 (100%)	164 (100%)	0	100	100
10	W	416/416 (100%)	413 (99%)	3 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	X	331/331 (100%)	331 (100%)	0	100	100
12	Y	334/334 (100%)	333 (100%)	1 (0%)	92	94
13	Z	257/257 (100%)	256 (100%)	1 (0%)	91	94
14	a	334/334 (100%)	334 (100%)	0	100	100
15	b	167/167 (100%)	166 (99%)	1 (1%)	86	92
16	c	252/252 (100%)	251 (100%)	1 (0%)	91	94
17	d	121/121 (100%)	120 (99%)	1 (1%)	81	89
18	e	63/63 (100%)	63 (100%)	0	100	100
19	f	579/714 (81%)	563 (97%)	16 (3%)	43	64
All	All	5619/5962 (94%)	5572 (99%)	47 (1%)	82	89

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	117	ASN
2	A	108	ASP
3	B	168	ASP
3	B	260	LEU
3	B	355	LEU
4	C	248	MET
4	C	287	LYS
4	C	293	MET
4	C	311	ILE
4	C	376	VAL
5	D	230	VAL
5	D	353	ASN
5	D	370	ILE
6	E	216	ARG
6	E	262	ASN
6	E	322	LYS
7	F	85	THR
7	F	168	TYR
7	F	180	ARG
7	F	323	ASN
8	U	397	THR
8	U	427	LEU
8	U	616	ARG
10	W	33	LYS
10	W	116	THR

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Mol	Chain	Res	Type
10	W	211	THR
12	Y	343	LEU
13	Z	90	ARG
15	b	25	ARG
16	c	282	ARG
17	d	190	LEU
19	f	39	LYS
19	f	89	MET
19	f	184	LEU
19	f	188	VAL
19	f	275	MET
19	f	314	TYR
19	f	391	LEU
19	f	460	ASP
19	f	473	ASN
19	f	493	ASN
19	f	565	ASN
19	f	569	LYS
19	f	639	LYS
19	f	696	LEU
19	f	745	LEU
19	f	788	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	100	ASN
1	G	117	ASN
2	A	165	GLN
2	A	314	ASN
3	B	131	HIS
3	B	193	GLN
3	B	241	ASN
3	B	315	GLN
4	C	22	GLN
5	D	65	GLN
5	D	133	HIS
5	D	175	GLN
5	D	286	GLN
5	D	301	GLN
5	D	353	ASN
6	E	45	ASN

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Mol	Chain	Res	Type
6	E	124	HIS
6	E	262	ASN
7	F	323	ASN
7	F	428	GLN
8	U	247	GLN
8	U	259	GLN
8	U	340	GLN
8	U	415	HIS
8	U	453	HIS
8	U	500	ASN
8	U	754	HIS
8	U	801	GLN
9	V	329	HIS
10	W	86	ASN
10	W	218	ASN
10	W	236	HIS
11	X	349	HIS
11	X	406	ASN
12	Y	178	ASN
12	Y	363	ASN
13	Z	189	GLN
13	Z	194	GLN
13	Z	282	ASN
14	a	35	HIS
14	a	152	HIS
14	a	264	ASN
14	a	288	HIS
15	b	29	GLN
15	b	34	ASN
15	b	76	HIS
15	b	99	HIS
15	b	149	ASN
16	c	183	HIS
16	c	241	ASN
16	c	254	ASN
17	d	141	GLN
19	f	180	GLN
19	f	301	HIS
19	f	327	ASN
19	f	405	HIS
19	f	475	ASN
19	f	493	ASN

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Mol	Chain	Res	Type
19	f	566	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	W	1
11	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	205:ILE	C	206:SER	N	3.19
1	X	311:ALA	C	312:GLU	N	3.16

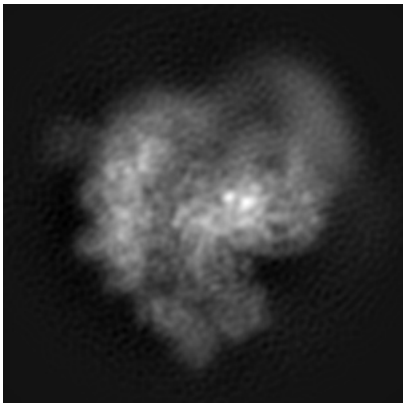
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8674. These allow visual inspection of the internal detail of the map and identification of artifacts.

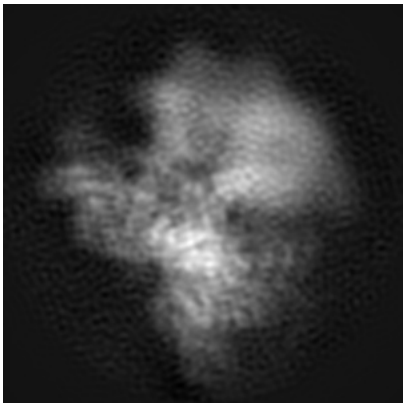
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

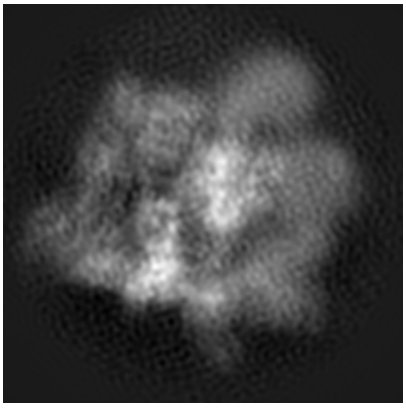
6.1.1 Primary map



X



Y

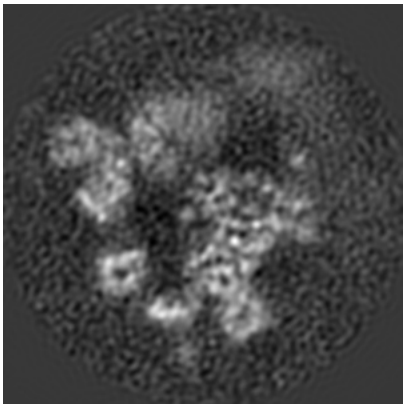


Z

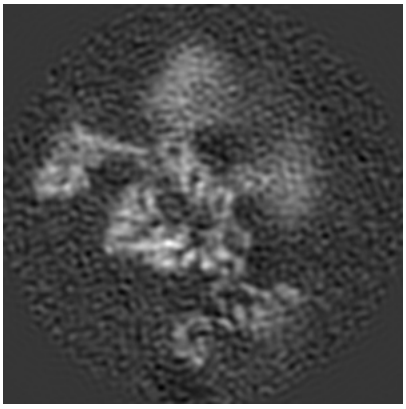
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

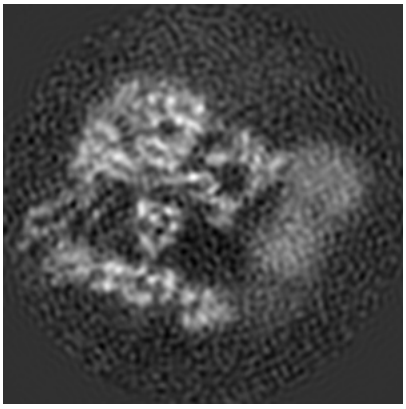
6.2.1 Primary map



X Index: 128



Y Index: 128

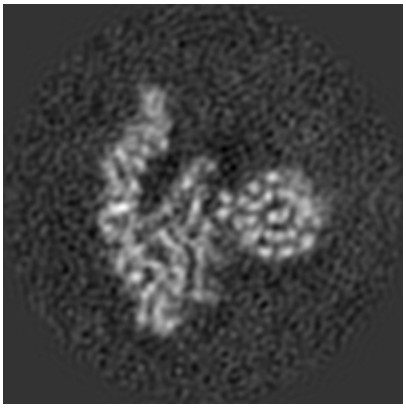


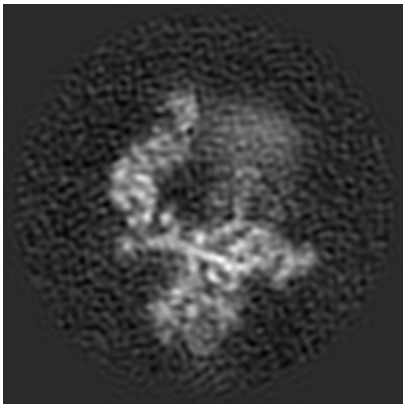
Z Index: 128

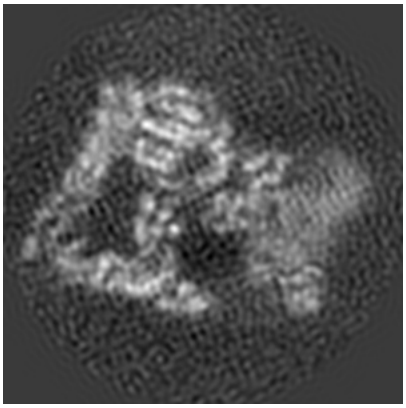
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 105

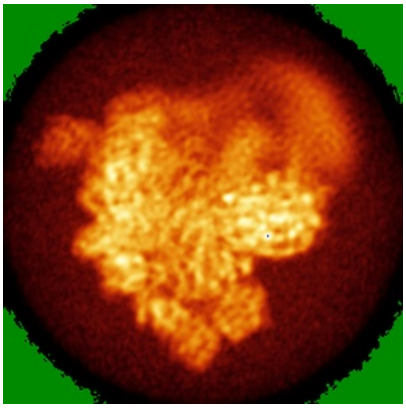

Y Index: 79

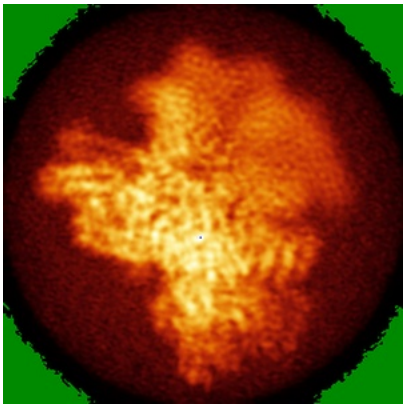

Z Index: 118

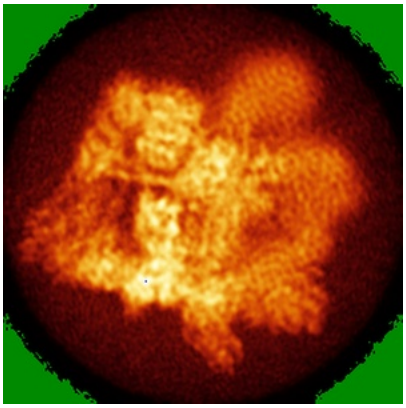
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

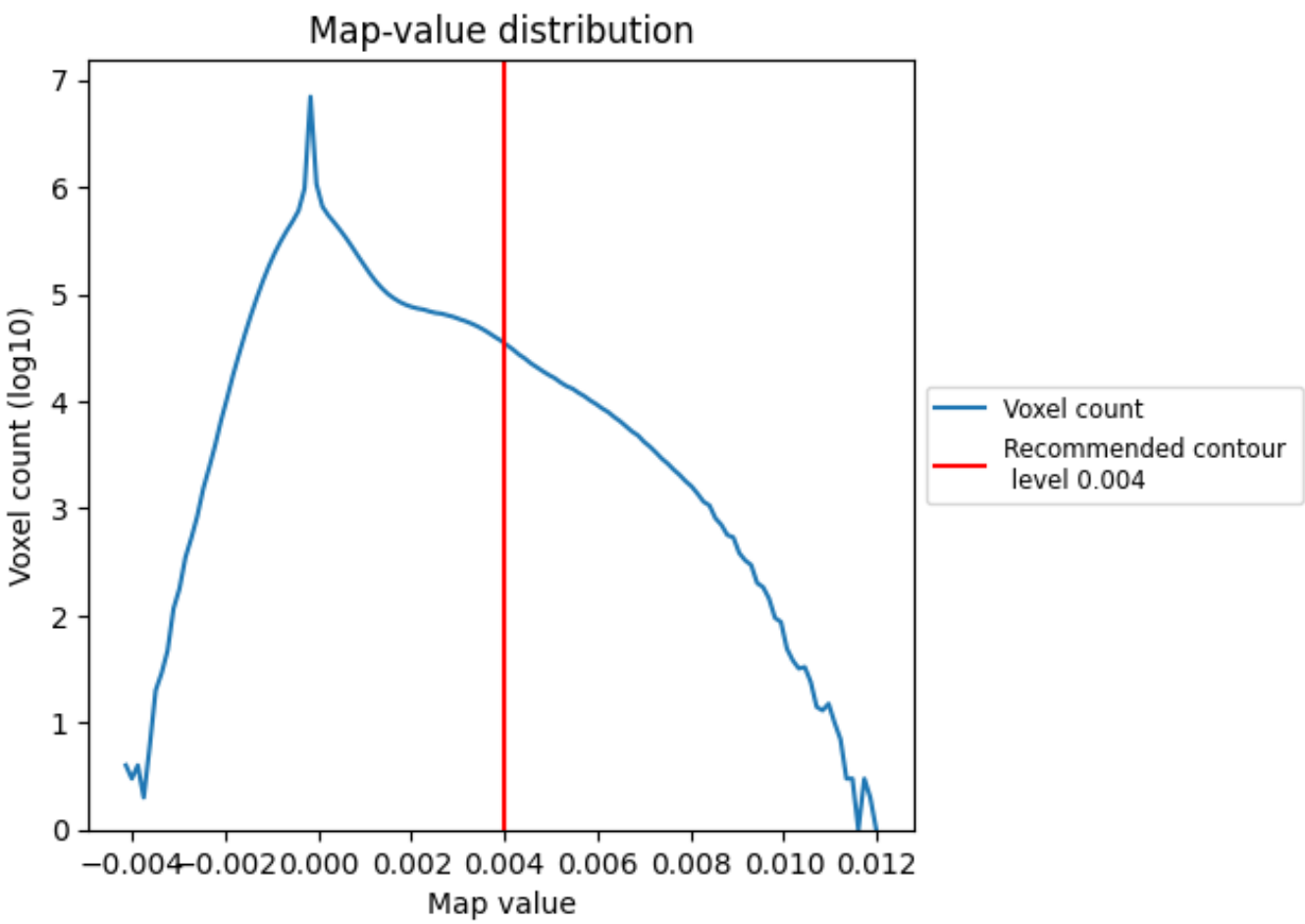
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

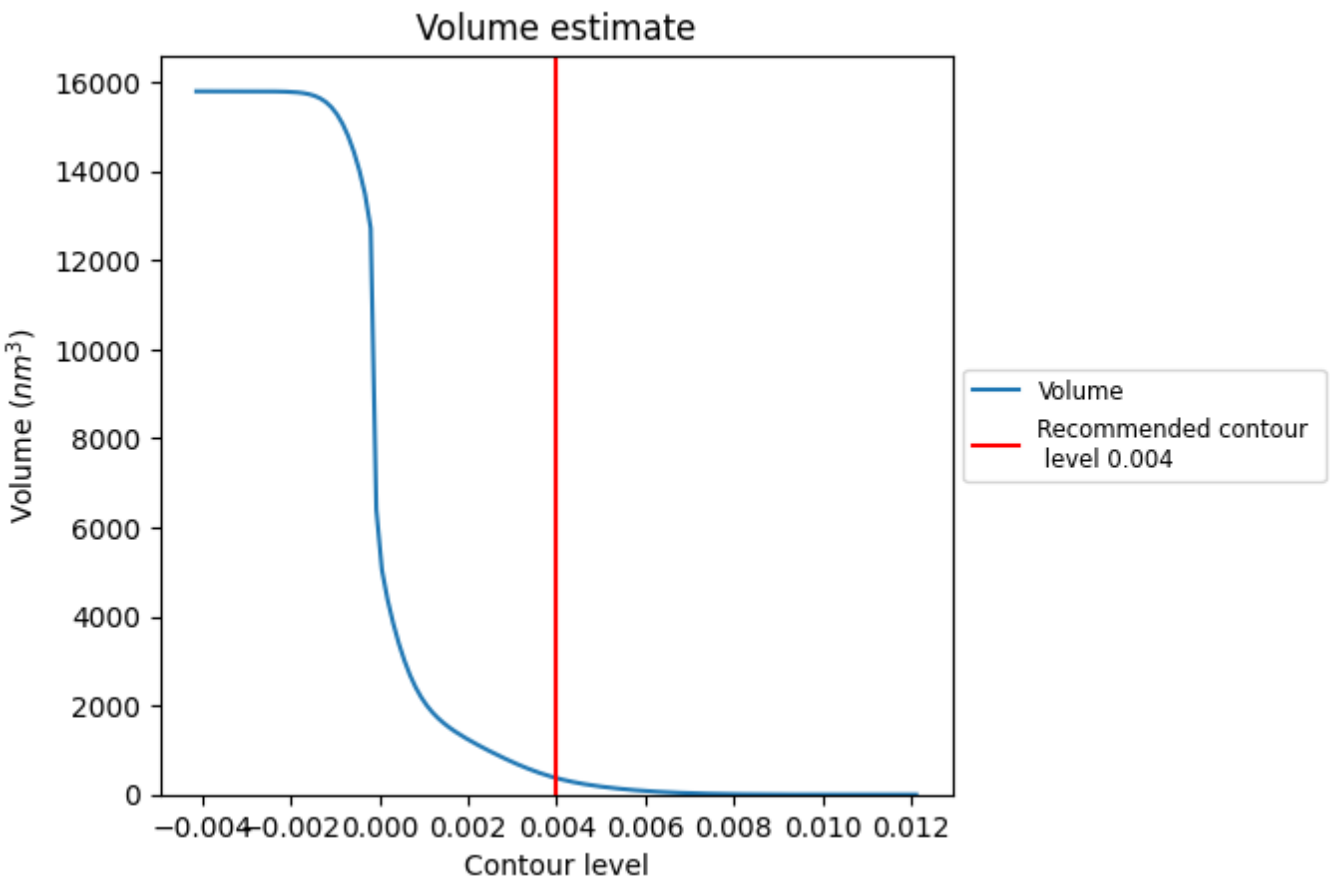
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

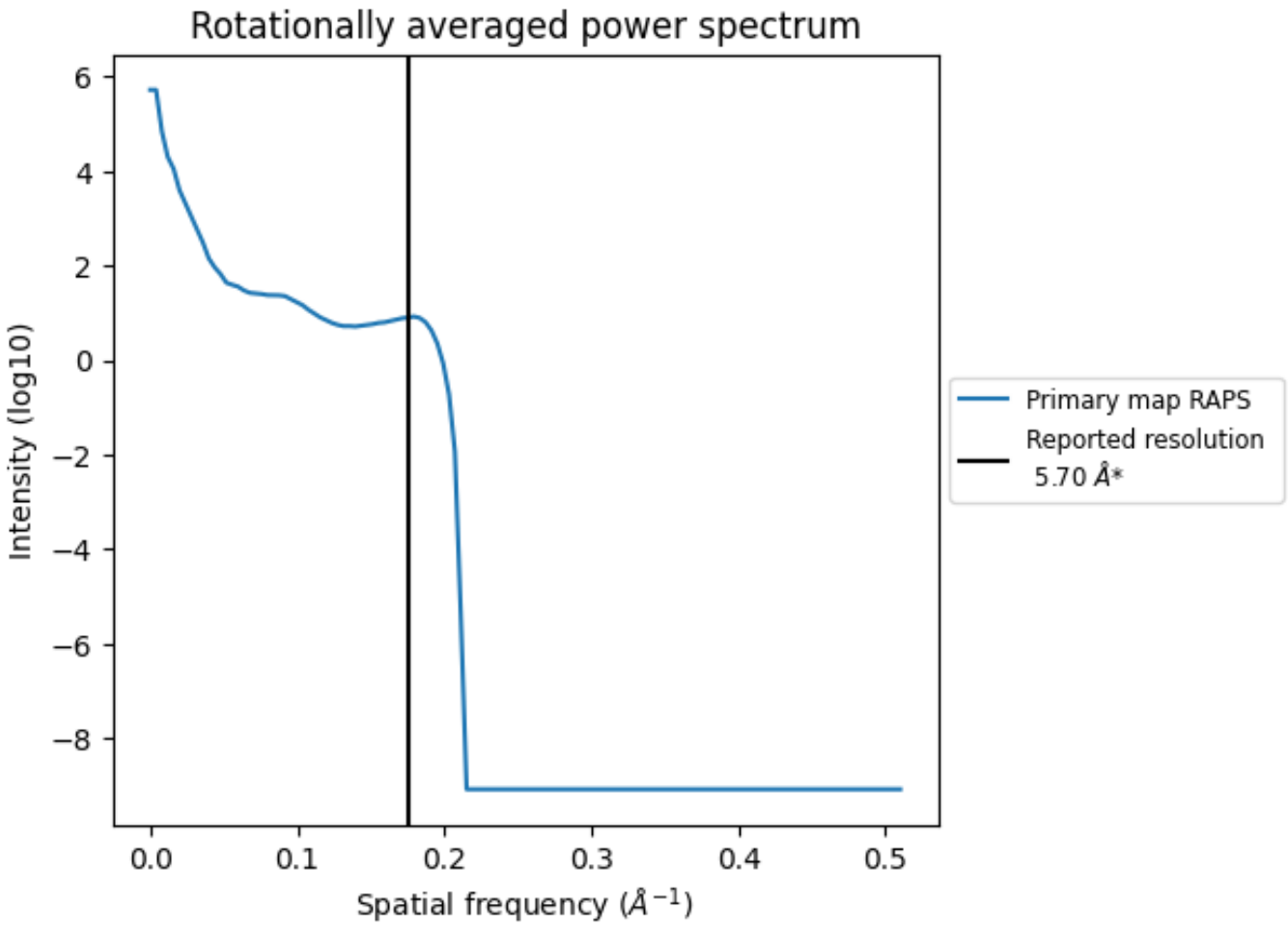
7.2 Volume estimate (i)



The volume at the recommended contour level is 369 nm^3; this corresponds to an approximate mass of 334 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.175 Å^{-1}

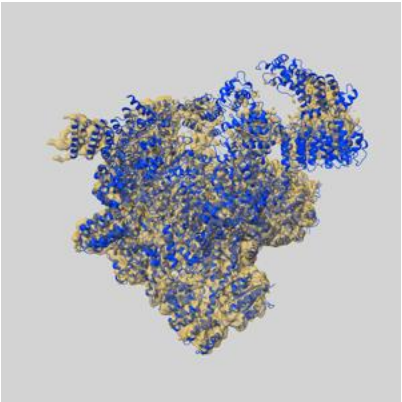
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

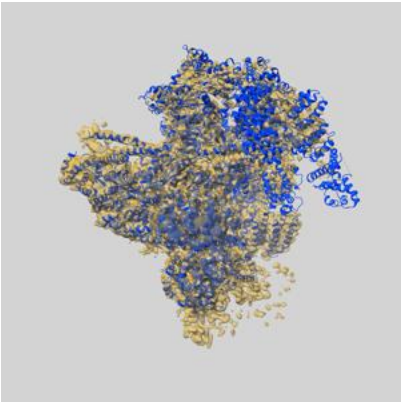
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8674 and PDB model 5VHF. Per-residue inclusion information can be found in section 3 on page 7.

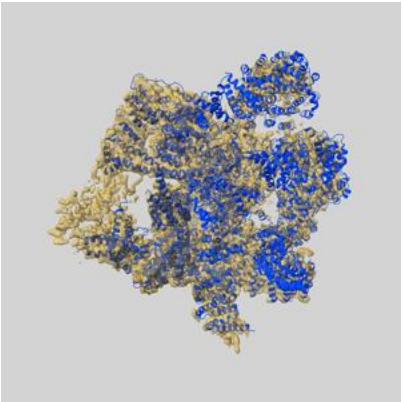
9.1 Map-model overlay (i)



X



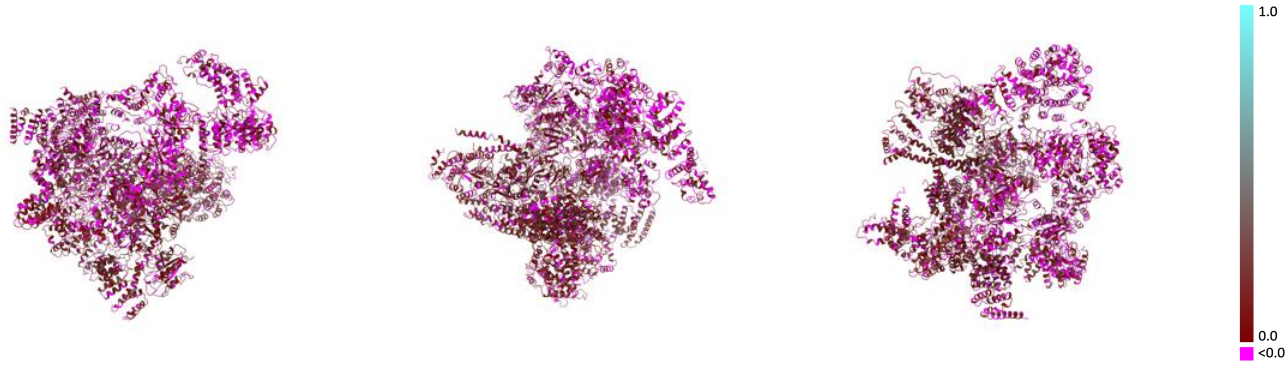
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

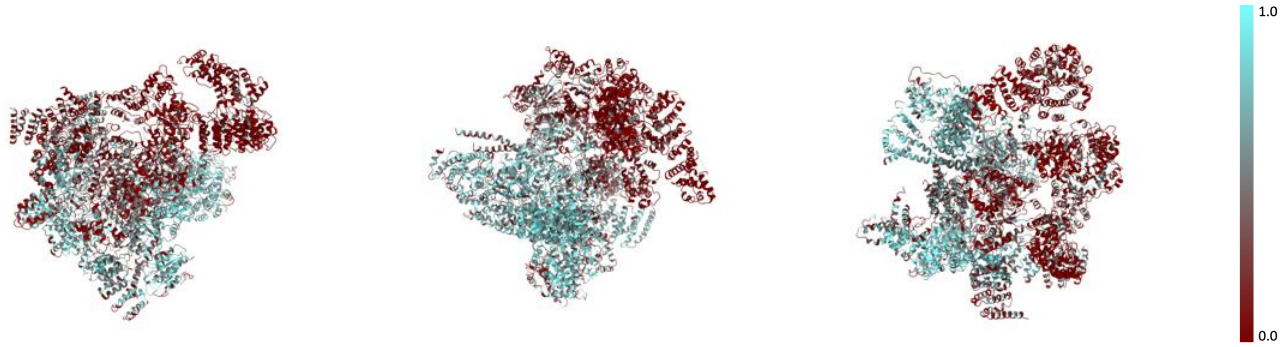
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

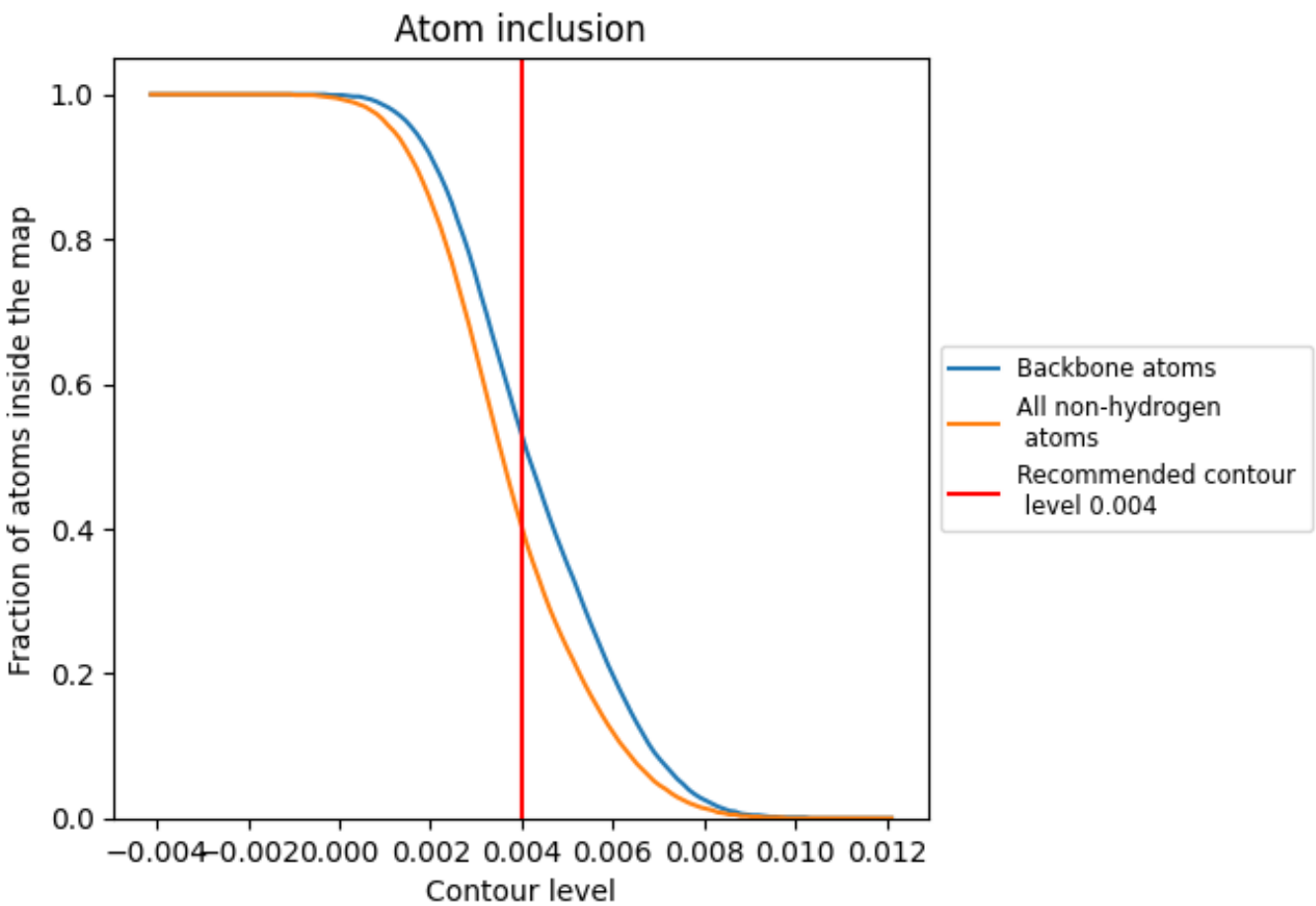
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4040	0.0860
A	0.2110	0.0390
B	0.1730	0.0260
C	0.2290	0.0480
D	0.2500	0.0730
E	0.2600	0.0650
F	0.2620	0.0620
G	0.0260	0.0200
U	0.6630	0.1360
V	0.5860	0.1130
W	0.5570	0.1070
X	0.4940	0.1080
Y	0.6730	0.1310
Z	0.5750	0.1310
a	0.5910	0.1310
b	0.5870	0.1110
c	0.5910	0.1460
d	0.4510	0.1050
e	0.4870	0.0640
f	0.0680	0.0160